

Amphibole Chemometers

Reference	Melt parameter	Output name	T-dependent?
Amphibole-only Chemometry. Function “<i>calculate_amp_only_melt_comps</i>” Returns all equations by default (need to specify T to get T-dependent equations)			
Ridolfi (2021)	ΔNNO	deltaNNO_Ridolfi21	X
	H_2O	H2O_Ridolfi21	X
Zhang et al. (2017)	SiO_2 (Eq 1)	SiO2_Eq1_Zhang17	X
	SiO_2 (Eq 2)	SiO2_Eq2_Zhang17	X
	SiO_2 (Eq 3)	SiO2_Eq3_Zhang17	✓
	SiO_2 (Eq 4)	SiO2_Eq4_Zhang17	X
	TiO_2 (Eq 5)	TiO2_Eq5_Zhang17	✓
	TiO_2 (Eq 6)	TiO2_Eq6_Zhang17	X
	FeO (Eq 7)	FeO_Eq7_Zhang17	X
	FeO (Eq 8)	FeO_Eq8_Zhang17	X
	MgO (Eq 9)	MgO_Eq9_Zhang17	X
	CaO (Eq 10)	CaO_Eq10_Zhang17	X
	CaO (Eq 11)	CaO_Eq11_Zhang17	X
	K_2O (Eq 12)	K2O_Eq12_Zhang17	X
	K_2O (Eq 13)	K2O_Eq13_Zhang17	X
	Al_2O_3 (Eq 14)	Al2O3_Eq14_Zhang17	X
Putirka (2016)	SiO_2 (Eq 10)	SiO2_Eq10_Put2016	✓

Amphibole Thermobarometers

Reference	Name in Thermobar	T-dependent?	P-dependent?	H ₂ O-dependent?
Amphibole-Liquid Barometry. Function “calculate_amp_liq_press”				
Putirka (2016)	P_Put2016_eq7a	X		✓
	P_Put2016_eq7b	X		✓ ^{1*}
	P_Put2016_eq7c	X		X
Amphibole-Liquid Thermometry. Function “calculate_amp_liq_temp”				
Putirka (2016)	T_Put2016_eq4b		X	✓
	T_Put2016_eq4a_amp_sat		X	✓ ^{1*}
	T_Put2016_eq9		X	✓ ^{1*}
Amphibole-only Barometry. Function “calculate_amp_only_press”				
Medard & Pennec (2022) ^{*2}	P_Medard2022_RidolfiSites P_Medard2022_LeakeSites P_Medard2022_MutchSites	X		X
Ridolfi and Renzulli (2012) & Ridolfi (2021)	P_Ridolfi2012_1a	X		X
	P_Ridolfi2012_1b	X		X
	P_Ridolfi2012_1c	X		X
	P_Ridolfi2012_1d	X		X
	P_Ridolfi2012_1e	X		X
	P_Ridolfi2021 ^{*3}	X		X
Mutch et al. (2016)	P_Mutch2016	X		X
Ridolfi et al. (2010)	P_Ridolfi2010	X		X
Hammerstrom & Zen (1986)	P_Hammarstrom1986_eq1	X		X
	P_Hammarstrom1986_eq2	X		X
	P_Hammarstrom1986_eq3	X		X
Hollister et al. (1987)	P_Hollister1987	X		X
Johnson & Rutherford (1989)	P_Johnson1989	X		X
Blundy et al. (1990)	P_Blundy1990	X		X
Schmidt (1992)	P_Schmidt1992	X		X
Anderson & Smith, 1995	P_Anderson1995	✓		X
Krawczynski et al. (2012)	P_Kraw2012	X		X
Amphibole-only Thermometry. Function “calculate_amp_only_temp”				
Putirka (2016)	T_Put2016_eq5		X	X
	T_Put2016_eq6		X	X
	T_Put2016_SiHbl		X	X
	T_Put2016_eq8		✓	X
Ridolfi and Renzuli, 2012	T_Ridolfi2012		✓	X
Amphibole-Plagioclase Thermometry. Function “calculate_amp_plag_temp”				
Holland and Blundy, 1994	T_HB1994_A T_HB1994_B		✓	X

✓^{1*} H₂O-dependence because of parameterization in terms of hydrous fractions, not a specific H₂O-term

^{*2} We provide 3 options for how to calculate Al^{VI}

^{*3} Equation P=“ P_Ridolfi2021” uses an algorithm to combine results of eq1a-1e

Clinopyroxene-Liquid Thermobarometers

Reference	Name in Thermobar	T-dependent?	P-dependent?	H ₂ O-dependent?
Clinopyroxene-Liquid Barometry. Function “calculate_cpx_liq_press”				
Putirka (1996)	P_Put1996_eqP1	✓		✗
	P_Put1996_eqP2	✓		✗
Putirka (2003)	P_Put2003	✓		✗
Putirka (2008)	P_Put2008_eq30	✓		✓
	P_Put2008_eq31	✓		✓
	P_Put2008_eq32c	✓		✓
Masotta et al. (2013) <i>recalibration of Putirka eqs. for alkali systems</i>	P_Mas2013_eqPalk1tex	✓		✗
	P_Mas2013_eqPalk2	✓		✗
	P_Mas2013_eqalk32c	✓		✓
Masotta et al. (2013)	P_Mas2013_Palk2012	✗		✓
Neave & Putirka (2017)	P_Neave2017	✓		✗
Petrelli et al. (2020)	P_Petrelli2020_Cpx_Liq* ¹	✗		✓
Jorgenson et al. (2022)	P_Jorgenson2022_Cpx_Liq* ¹	✗		✗
Clinopyroxene-Liquid Thermometry. Function “calculate_cpx_liq_temp”				
Putirka (1996)	T_Put1996_eqT1		✗	✗
	T_Put1996_eqT2		✓	✗
Putirka (1999)	T_Put1999		✓	✗
Putirka (2003)	T_Put2003		✓	✗
Putirka (2008)	T_Put2008_eq33		✓	✓
Masotta et al. (2013) <i>Recalibration of Putirka eqs. for alkali systems</i>	T_Mas2013_eqTalk1		✗	✗
	T_Mas2013_eqTalk2		✓	✗
	T_Mas2013_eqalk33		✓	✓
Masotta et al. (2013)	T_Mas2013_Talk2012		✗	✓
Brugman & Till (2019)	T_Brug2019		✗	✗
Petrelli et al. (2020)	T_Petrelli2020_Cpx_Liq* ¹		✗	✓
Jorgenson et al. (2022)	T_Jorgenson2022_Cpx_Liq* ¹		✗	✗

Clinopyroxene-only Thermobarometers

Reference	Name in Thermobar	T-dependent?	P-dependent?	H ₂ O-dependent?
Clinopyroxene-only Barometry. Function "calculate_cpx_only_press"				
Putirka (2008)	P_Put2008_eq32a	✓		✗
	P_Put2008_eq32b	✓		✓
Petrelli et al. (2020) *our adaptations	P_Petrelli2020_Cpx_only* ¹	✗		✗
	P_Petrelli2020_Cpx_only_withH2O*	✗		✓
Wang et al. (2021)	P_Wang2021_eq1	✗		✗
Jorgenson et al. (2022)	P_Jorgenson2022_Cpx_only* ¹	✗		✗
Clinopyroxene-only Thermometry. Function "calculate_cpx_only_temp"				
Putirka (2008)	T_Put2008_eq32d		✓	✗
	T_Put2008_eq32d_subsol		✓	✗
Wang et al. (2021)	T_Wang2021_eq2		✗	✓
Jorgenson et al. (2022)	T_Jorgenson2022_Cpx_only* ¹		✗	✗

Liquid-only thermometry

Function: "calculate_liq_only_temp"

Reference	Name in Thermobar	P-dependent?	H ₂ O-dependent?
Olivine-Sat Liquids			
Putirka (2008)	T_Put2008_eq13	✗	✗
	T_Put2008_eq14	✗	✓
	T_Put2008_eq15	✓	✓
Helz & Thornber, (1987)	T_Helz1987_MgO	✗	✗
Shea et al. (2022)	T_Shea2022_MgO	✗	✗
Montierth (1995)	T_Montierth1995_MgO	✗	✗
Sugawara (2000)	T_Sug2000_eq1	✗	✗
	T_Sug2000_eq3_ol	✓	✗
	T_Sug2000_eq6a	✓	✗
	T_Sug2000_eq6a_H7a	✓	✓
Beattie (1993)	T_Beatt93_BeattDMg	✓	✗
	T_Beatt93_BeattDMg_HerzCorr	✓	✗
Putirka (2008)	T_Put2008_eq19_BeattDMg	✓	✗
	T_Put2008_eq21_BeattDMg	✓	✓
	T_Put2008_eq22_BeattDMg	✓	✓
Cpx-Sat Liquids			
Putirka (2008)	T_Put2008_eq34_cpx_sat	✓	✓
Putirka (1999)	T_Put1999_cpx_sat	✓	✗
Sugawara (2000)	T_Sug2000_eq3_cpx	✓	✗
	T_Sug2000_eq3_pig	✓	✗
	T_Sug2000_eq6b	✓	✗
	T_Sug2000_eq6b_H7b	✓	✓
Opx-Sat Liquids			
Putirka (2008)	T_Put2008_eq28b_opx_sat	✓	✓
Sugawara (2000)	T_Sug2000_eq3_opx	✓	✗
Beattie (1993)	T_Beatt1993_opx	✓	✗
Amp-Sat Liquids			
Putirka (2008)	T_Put2016_eq3_amp_sat	✗	✓*
Molina (2015)	T_Molina2015_amp_sat	✗	✗
Fspar-Sat Liquids			
Putirka (2005)	T_Put2005_eqD_plag_sat	✓	✓
Putirka (2008)	T_Put2008_eq26_plag_sat	✓	✓
	T_Put2008_eq24c_kspar_sat	✓	✓
OI-Cpx-Plag Sat Liquids			
Putirka (2008)	T_Put2008_eq16	✓	✗
Helz & Thornber (1987)	T_Helz1987_CaO	✗	✗

Orthopyroxene Thermobarometers

Reference	Name in Thermobar	T-dependent?	P-dependent?	H ₂ O-dependent?
Orthopyroxene-Liquid Barometry. Function "calculate_opx_liq_press"				
Putirka (2008)	P_Put2008_eq29a	✓		✓
	P_Put2008_eq29b	✓		✓
Putirka Supplement New "Global" calibrations	P_Put_Global_Opx	✗		✗
	P_Put_Felsic_Opx	✗		✗
Orthopyroxene-Liquid Thermometry. Function "calculate_opx_liq_temp"				
Putirka (2008)	T_Put2008_eq28a		✓	✓
	T_Put2008_eq28b_opx_sat		✓	✓
Orthopyroxene-only Barometry. Function "calculate_opx_only_press"				
Putirka (2008)	P_Put2008_eq29c	✓		✗

Orthopyroxene-Clinopyroxene Thermobarometers

Reference	Name in Thermobar	T-dependent?	P-dependent?	H ₂ O-dependent?
Orthopyroxene-Clinopyroxene Barometry. Function “calculate_cpx_opx_press”				
Putirka (2008)	P_Put2008_eq38	✗		✗
	P_Put2008_eq39	✓		✗
Orthopyroxene-Clinopyroxene Thermometry. Function “calculate_cpx_opx_press”				
Putirka (2008)	T_Put2008_eq36		✓	✗
	T_Put2008_eq37		✓	✗
Brey and Kohler (1990)	T_Brey1990		✓	✗
Wells (1977)	T_Wells1977		✗	✗
Wood and Banno (1973)	T_Wood1973		✗	✗

Feldspar Thermometers, Barometers and Hygrometers

Phase	Reference	Name in Thermobar	T-dependent?	P-dependent?	H ₂ O-dependent?
Feldspar-Liquid thermometry. Function "calculate_fspar_liq_temp"					
Plag-Liq	Putirka (2008)	T_Put2008_eq23		✓	✓
		T_Put2008_eq24a		✓	✓
Kspar-Liq	Putirka (2008)	T_Put2008_eq24b		✓	✗
Feldspar-Liquid barometry. Function "calculate_fspar_liq_press"					
Plag-Liq	Putirka (2008)	P_Put2008_eq25	✓		✗
Feldspar-Liquid hygrometry. Function "calculate_fspar_liq_hygr"					
Plag-Liq	Putirka (2008)	H_Put2008_eq25b	✓	✓	
	Putirka (2005)	H_Put2005_eqH	✓	✗	
	Waters & Lange (2015)	H_Waters2015	✓	✓	
	Masotta et al. (2019)	H_Masotta2019	✓	✗	
Plagioclase-Alkali Feldspar thermometry. Function "calculate_plag_kspar_temp"					
Plag-Kspar	Putirka (2008)	T_Put2008_eq27a		✓	✗
		T_Put2008_eq27b		✓	✗
		T_Put_Global_2Fspar		✓	✗

Garnet Thermometers and Barometers

Reference	Name in Thermobar	T-dependent?	P-dependent?	H ₂ O-dependent?
Garnet-only thermometry. Function “calculate_gt_only_temp”				
Ryan et al. (1996)	T_Ryan1996		✗	✗
Canil et al. (1999)	T_Canil1999		✗	✗
Sudholz et al. (2021)	T_Sudholz2021		✗	✗
Garnet-only barometry Function “calculate_gt_only_press”				
Ryan et al. (1996)	P_Ryan1996	✓		✗

Other Garnet Functions

Garnet classification of Griffin et al. (2002)	"garnet_CARP_class_Griffin2002"
Cr-pyrope classification of Grutter et al. (2004)	"garnet_class_Grutter2004"
Ca-Cr classification of Cr-pyrope of Griffin et al. (2002)	"garnet_ca_cr_class_Griffin2002"
Y-Zr Classification of Cr-pyrope of Griffin et al. (2002)	"y_zr_classification_Griffin2002"
Ol Mg# from Cr-pyrope (Gaul et al. 2000)	"calculate_ol_mg"
Calculate Al ₂ O ₃ of whole-rock from Cr-pyrope (after O'Reilly et al. 2006)	"calculate_al2O3_whole_rock"

Olivine Thermometers and Hygrometers

Reference	Name in Thermobar	T-dependent?	P-dependent?	H ₂ O-dependent?
Olivine-Liquid thermometry. Function “calculate_ol_liq_temp”				
Putirka (2008)	T_Put2008_eq19		✓	✗
	T_Put2008_eq21		✓	✓
	T_Put2008_eq22		✓	✓
Beattie (1993)	T_Beatt93_ol		✓	✗
	T_Beatt93_ol_HerzCorr		✓	✗
Sisson and Grove (1992)	T_Sisson1992		✓	✗
Pu et al. (2017)	T_Pu2017		✗	✗
Pu et al. (2021)	T_Pu2021		✓	✗
Olivine-Liquid hygrometers. Function “calculate_ol_liq_hygr”				
Gavrilenko et al. (2016)	H_Gavr2016	✗	✗	
Olivine-Spinel thermometry. Function “calculate_ol_sp_temp”				
Coogan et al. (2014)	T_Coogan2014		✗	✗
Wan et al. (2008)	T_Wan2008		✗	✗